

**WE CLAIM:**

- 1           1.     A mass spectrometer system, comprising:  
2                     a data acquisition unit operable to sense and generate raw data indicative of  
3 masses of particles; and  
4                     a computing unit in communication with said data acquisition unit and configured  
5 to receive the raw data from said data acquisition unit and transform the raw data into  
6 transformed data having a hierarchical data format for use at multiple resolutions.
- 1           2.     The mass spectrometer system according to claim 1, wherein said computing unit  
2 is further configured to compress the transformed data.
- 1           3.     The mass spectrometer system according to claim 2, wherein said computing unit  
2 uses a lossless compression technique to compress the transformed data.
- 1           4.     The mass spectrometer system according to claim 1, wherein said computing unit  
2 is further configured to identify noise in the transformed data.
- 1           5.     The mass spectrometer system according to claim 4, wherein said computing unit  
2 is further configured to reduce the noise in the transformed data.

6. The mass spectrometer system according to claim 1, further comprising a display unit in communication with said computing unit and operable to display the transformed data at multiple resolutions.

7. The mass spectrometer system according to claim 1, wherein said computing unit utilizes a wavelet transformation having filters that transform the raw data into the transformed data.

8. The mass spectrometer system according to claim 7, wherein said processing unit is further operable to optimize the filters used in the wavelet transformation.

9. The mass spectrometer system according to claim 8, wherein said processing unit is further operable to generate multiple sub-datasets from the raw data.

10. The mass spectrometer system according to claim 9, wherein the multiple datasets include a first dataset formed of odd indexed elements of the raw data and a second dataset formed of even indexed elements of the raw data.

11. The mass spectrometer system according to claim 9, wherein said processing unit is configured to determine classifiers for optimizing the filters.

12. The mass spectrometer system according to claim 11, wherein the classifiers include classifiers for scales and differences.

1           13.     The mass spectrometer system according to claim 11, wherein said processing  
2     unit is further configured to generate a rule set for optimizing the filters.

1           14.     The mass spectrometer system according to claim 13, wherein the rule set  
2     includes a function for taking a maximum of an argument.

1           15.     The mass spectrometer system according to claim 13, wherein said processing  
2     unit is further configured to obtain an estimate for an optimal predictor based on the classifiers to  
3     produce an interpolation point from the transformed data.

1           16.     The mass spectrometer system according to claim 1, wherein said processing unit  
2     further includes a decoder to decode the transformed data utilizing the rule set.

1           17.     A method for storing mass spectrometer data, said method comprising:  
2                     receiving raw data indicative of masses of particles produced by a mass  
3 spectrometer; and  
4                     transforming the raw data into transformed data having a hierarchical data format  
5 for use at multiple resolutions.

1           18.     The method according to claim 17, further comprising compressing the  
2 transformed data.

1           19.     The method according to claim 18, wherein said compressing the transformed  
2 data is performed using a lossless compression technique.

1           20.     The method according to claim 17, further comprising identifying noise in the  
2 transformed data.

1           21.     The method according to claim 20, further comprising reducing the noise in the  
2 transformed data.

1           22.     The method according to claim 21, further comprising compressing the  
2 transformed data having reduced noise.

1           23.     The method according to claim 17, further comprising displaying the transformed  
2 data at multiple resolutions.

1           24.     The method according to claim 17, wherein said transforming includes performing  
2     a wavelet transformation on the raw data to produce the transformed data having a hierarchical  
3     data format.

1           25.     The method according to claim 17, further comprising decoding the transformed  
2     data.

1           26.    A mass spectrometer system, comprising:

2                   means for receiving raw data indicative of masses of particles; and

3                   means for transforming the raw data into transformed data having a hierarchical  
4 data format for use at multiple resolutions, said means for transforming being in communication  
5 with said means for generating.

1           27.    The method according to claim 26, further comprising means for compressing the

2 transformed data.

1           28.    The method according to claim 26, further comprising means for identifying noise

2 in the transformed data.

1           29.    The method according to claim 28, further comprising means for reducing the

2 identified noise in the transformed data.

1           30.     The method according to claim 29, further comprising means for compressing the  
2 transformed data having reduced noise.

1           31.     The method according to claim 26, further comprising means for displaying the  
2 transformed data at multiple resolutions.

1           32.     The method according to claim 26, further comprising means for decoding the  
2 transformed data.

1           33.     A method for processing mass spectrometry data, said method comprising:  
2                     receiving a request to perform an operation utilizing at least a portion of  
3 transformed data resulting from a transformation of raw data generated by a mass spectrometer,  
4 the transformed data having a hierarchical data format for use at multiple resolutions;  
5                     accessing the transformed data;  
6                     selecting parameters to use for a selected resolution of the transformed data;  
7                     producing a transformed dataset at the selected resolution from the transformed  
8 data as a function of the selected parameters; and  
9                     performing the requested operation on the transformed dataset at the selected  
10 resolution to generate a result for the operation based on the transformed dataset at the selected  
11 resolution in response to said receiving the request.

1           34.     The method according to claim 33, wherein said receiving the request includes  
2 receiving a request to compare a test dataset with the transformed data.

1           35.     The method according to claim 33, wherein said receiving the request includes  
2 receiving a search request for transformed data having certain properties.

1           36.     The method according to claim 33, wherein said receiving the request includes  
2 receiving a request to compress the transformed data.



1           37.     The method according to claim 33, wherein said receiving the request includes  
2 receiving a request to identify noise contained in the transformed data.

1           38.     The method according to claim 37, wherein said receiving the request includes  
2 receiving a request to identify chemical noise contained in the transformed data.

1           39.     The method according to claim 37, further comprising receiving a request to  
2 suppress the noise.

1           40.     The method according to claim 33, further comprising decoding the transformed  
2 data at the selected resolution.

1           41.     A system for processing mass spectrometry data, said system comprising:

2                     a storage unit operable to store transformed data resulting from a transformation  
3 of raw data generated by a mass spectrometer, the transformed data having a hierarchical data  
4 format for use at multiple resolutions; and

5                     a processing unit in communication with said storage unit and configured to:

6                             receive a request to perform an operation utilizing at least a portion of  
7 transformed data resulting from a transformation of raw data generated by a mass  
8 spectrometer, the transformed data having a hierarchical data format for use at multiple  
9 resolutions;

10                            access the transformed data;

11                           select parameters to use for a selected resolution of the transformed data;

12                           produce a transformed dataset at the selected resolution from the  
13 transformed data as a function of the selected parameters; and

14                           perform the requested operation on the transformed dataset at the selected  
15 resolution to generate a result for the operation based on the transformed dataset at the  
16 selected resolution in response to receiving the request.

1           42.     The system according to claim 41, wherein the operation includes comparing a  
2 test dataset with the transformed data.

1           43.     The system according to claim 41, wherein the operation includes searching for  
2 transformed data having certain properties.

1           44.     The system according to claim 41, wherein said processing unit is further operable  
2     to compress the transformed data.

1           45.     The system according to claim 41, wherein the operation includes identifying  
2     noise contained in the transformed data.

1           46.     The system according to claim 45, wherein the noise is chemical noise.

1           47.     The system according to claim 45, wherein the operation includes suppressing the  
2     noise.

1           48.     The system according to claim 41, wherein said processing unit is further operable  
2     to decode the data at the selected resolution.

1           49.    A method for formatting data measured by a mass spectrometer, said method  
2 comprising:  
3                receiving raw data sampled by the mass spectrometer;  
4                generating an interpolating polynomial of order  $p$  for use in generating  
5 coefficients;  
6                splitting the raw data into multiple raw subsample datasets;  
7                generating a first vector of optimal classification indices on scales;  
8                generating a second vector of optimal classification indices on differences;  
9                generating a ruleset matrix based on an indicator function;  
10               generating a predictor as a function of the ruleset, first vector, and second vector;  
11               based on each predictor, updating the second raw subsample dataset utilizing the  
12 coefficients; and  
13               outputting the ruleset matrix, first raw subsample dataset, and updated second raw  
14 subsample dataset for use of the data measured by the mass spectrometer at multiple resolutions.

1           50.    The method according to claim 49, wherein said splitting of the raw data includes  
2 forming two raw subsample datasets, a first dataset including odd indexed raw data elements and  
3 a second dataset including even indexed raw data elements.

1           51.    The method according to claim 49, wherein said generating the ruleset matrix is  
2 performed by utilizing a maximum of an argument (MAXARG) function.

1           52.    The method according to claim 49, further comprising compressing the datasets.

1           53.    The method according to claim 49, further comprising:

2                identifying noise included in the raw data; and

3                suppressing the identified noise.

1           54.    A system for formatting data measured by a mass spectrometer, said system  
2 comprising:  
3                   means for receiving raw data sampled by the mass spectrometer;  
4                   means for generating an interpolating polynomial of order  $p$  for use in generating  
5 coefficients and in communication with said means for receiving;  
6                   means for splitting the raw data into multiple raw subsample datasets, and in  
7 communication with said means for receiving;  
8                   means for generating a first vector of optimal classification indices on scales, and  
9 in communication with said means for splitting to receive the multiples raw subsample datasets  
10 to generate the first vector;  
11                  means for generating a second vector of optimal classification indices on  
12 differences, and in communication with said means for splitting to receive the multiple raw  
13 subsample datasets to generate the second vector;  
14                  means for generating a ruleset matrix based on an indicator function, and in  
15 communication with said means for splitting to receive the multiple raw subsample datasets to  
16 generate the ruleset matrix;  
17                  means for generating a predictor as a function of the ruleset matrix, first vector,  
18 and second vector, operable to receive the ruleset matrix first vector, and second vector;  
19                  means for updating the second raw subsample dataset utilizing the coefficients  
20 and in response to each predictor; and

21 means for outputting the ruleset matrix, first raw subsample dataset, and updated  
22 second raw subsample dataset for use of the data measured by the mass spectrometer at multiple  
23 resolutions.

1 55. The system according to claim 54, further comprising means for compressing the  
2 datasets in communication with said means for outputting.

1 56. The system according to claim 54, further comprising:  
2 means for identifying noise included in the raw data and operable to receive the  
3 raw data or the multiple raw subsample datasets; and  
4 means for suppressing the identified noise in communication with said means for  
5 identifying noise.

1           57.    A method for formatting data measured by a mass spectrometer, said method  
2 comprising:  
3                   receiving a dataset containing mass spectrometer data;  
4                   performing a wavelet transformation on the mass spectrometer data to generate a  
5 transformed dataset; and  
6                   storing the transformed dataset.

1           58.    The method according to claim 57, further comprising compressing the  
2 transformed dataset.

1           59.    The method according to claim 57, further comprising suppressing noise  
2 contained in the transformed dataset.

1           60.    The method according to claim 57, further comprising suppressing noise  
2 contained in the transformed dataset.

1           61.    The method according to claim 57, further comprising optimizing filters over  
2 localized regions.

1           62.    The method according to claim 61, further comprising generating a ruleset for  
2 performing predictions in interpolating datapoints.



1           63.     A system for formatting data measured by a mass spectrometer, said system  
2 comprising:  
3                   a processor operable (i) to receive a dataset containing mass spectrometer data and  
4 (ii) to perform a wavelet transformation on the mass spectrometer data to generate a transformed  
5 dataset; and  
6                   a storage unit in communication with said processor and operable to receive and  
7 store the transformed dataset communicated from said processor.

1           64.     The system according to claim 63, wherein said processor is further operable to  
2 compress the transformed dataset.

1           65.     The system according to claim 64, wherein said processor is further operable to  
2 suppress the noise contained in the transformed dataset.

1           66.     The system according to claim 63, wherein said processor is further operable to  
2 suppress the noise contained in the transformed dataset.

1           67.     The method according to claim 63, further comprising optimizing filters over  
2 localized regions.

1           68.     The method according to claim 67, further comprising generating a ruleset for  
2 performing predictions for interpolating datapoints.